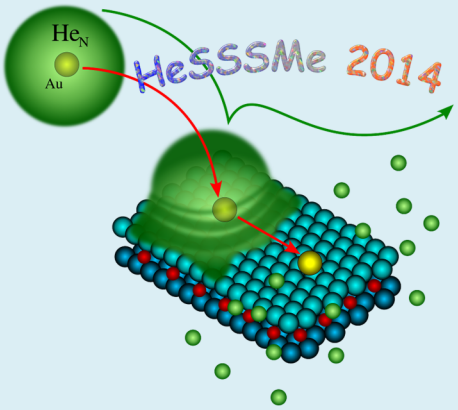
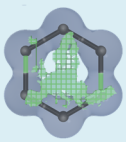
Workshop “Helium-mediated Synthesis, Soft-landing and Spectroscopy of Metal Nanoparticles on Surfaces”

October 10-11, 2014
CSIC, Madrid, Spain



BOOK OF ABSTRACTS



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LABORATOIRE DE MODÉLISATION ET SIMULATION MULTI ÉCHELLE
Sous la co-tutelle de :
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POSTER PRESENTATIONS

Accurate global potentials for the interaction between rare gases and graphene-based surfaces. Diffraction and quasibound states.

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The interaction between rare-gas atoms with graphene type surfaces is a topic of great interest given the many applications of these materials that can be foreseen. For example, some porous derivatives, have been proposed as a nano-scale membrane which could be used as an atmospheric nanofilter[1]. For most of these studies it is necessary not only a reliable and accurate description of the interaction potential but it is also fundamental to obtain a convenient parametrization to support dynamical studies on the physisorption of atoms or molecules.

We report reliable global potentials for the physisorption of rare gases with graphene and graphite surfaces amenable for a variety of dynamics simulations[2]. An atom-bond pairwise additive form of the potential is used, where the interaction pairs are constituted by the Rg atom (Rg= He, Ne, Ar, Kr) and the C-C bonds of the graphene sheet(s). The parameters of the atom-bond pair potential, derived from the polarizability of the interacting partners, are fine-tuned exploiting calculations of the prototypical Rg-coronene system through high level electronic structure methods. The atom-graphene/graphite potential is further expanded in a Fourier series that only requires a small number of corrugation terms.

Our results results are found to compare well with previous data[3] regarding well depths and equilibrium distances at different adsorption sites. Diffraction intensities are more sensitive and results based on Close-Coupled calculations[4] are shown for the system He-graphene.

References:

[1] M. Bartolomei et al. "Penetration Barrier of Water through Graphynes' Pores: First-Principles Predictions and Force Field Optimization". JOURNAL OF PHYSICAL CHEMISTRY LETTERS. **5** , 751 (2014).
[2] M. Bartolomei et al. "Global Potentials for the Interaction between Rare Gases and Graphene-Based Surfaces: An Atom-Bond Pairwise Additive Representation". JOURNAL OF PHYSICAL CHEMISTRY C. **117**, 10512 (2013).
[3] G. Vidali et al., *Surf. Sci. Rep.,* **12**, 133 (1991).
[4] M. I. Hernández et al."Lifetimes of Selective-Adsorption Resonances in Atomo-Surface Elastic Scattering". PHYSICAL REVIEW B. **49**, 8300 (1994).

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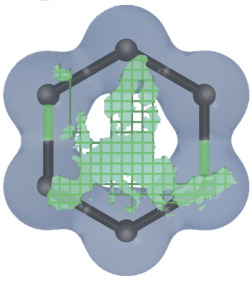


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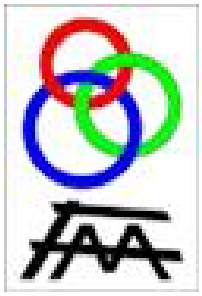

Program

Friday 10/10		
9:20 – 9:50	Registration	
9:50 – 10:00	Opening of HESSSME-2014	
	Session I	**Chair**: Pablo Villareal Herrán, CSIC (Spain)
10:00 – 10:35	I1	Wolfgang E. Ernst
10:35 – 11:10	I2	Robert Hinde
11:10 – 11:45	I3	Jordi Boronat
11:45 – 12:15	**Coffee break**	
	Chair: Marius Lewerenz, UPEM (France)	
12:15 – 12:50	I4	Pierre-Nicholas Roy
12:50 – 13:25	I5	Nadine Halberstadt
13:25 – 13:40	S1	Antonio Sarsa
14:00 – 15:30	**Lunch**	
	Session II	**Chair**: Salvador Montero, CSIC (Spain)
15:30 – 16:05	I6	Frank Steinkemeier
16:05 – 16:20	S2	Massimo Mella
16:20 – 16:35	PP	Antonio Leal
16:35 – 16:50	PP	Arnau Vilà
16:50 – 18:25	**Coffee break/Poster Discussions**	
	Chair: Francesco Ancilotto, Padova University (Italy)	
18:25 – 19:00	I7	Céline Léonard
19:00 – 19:35	I8	Claron J. Ridge
20:00 – 22:30	**Walk to Downtown of Madrid**	

Saturday 11/10		
	Session III	**Chair**: Octavio Roncero, CSIC (Spain)
9:40 – 10:15	I9	Andrew M. Ellis
10:15 – 10:50	I10	Lauri Halonen
10:50 – 11:05	S3	Alexandre Zanchet
11:05 – 11:20	S4	Lyudmila Moskaleva
11:20 – 11:45	**Coffee break**	
	Chair: José Campos Martínez, CSIC (Spain)	
11:45 – 12:00	S5	Gilberte Chambaud
12:00 – 12:35	I11	Kari Laasonen
12:35 – 13:10	I12	Pablo García González
13:10 – 14:00	Final remarks	
14:00 – 15:30	**Lunch**	
15:30 –	Informal discussions	